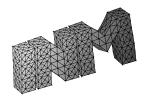
Technische Universität Graz



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ANALYSIS AND REGULARIZATION OF PROBLEMS IN DIFFUSE OPTICAL TOMOGRAPHY

HERBERT EGGER^{\dagger} AND MATTHIAS SCHLOTTBOM^{\ddagger}

ABSTRACT. In this paper we consider the regularization of the inverse problem of diffuse optical tomography by standard regularization methods with quadratic penalty terms. We therefore investigate in detail the properties of the associated forward operators, and derive continuity and differentiability results, which are based on derivation of $W^{1,p}$ regularity results for the governing elliptic boundary value problems. We then show that Tikhonov regularization can be applied for a stable solution, and that the standard convergence and convergence rates results hold. Our analysis also ensure convergence of iterative regularization methods, which are important from a practical point of view.

1. INTRODUCTION

Diffuse optical tomography is a non-invasive imaging technique that utilizes near-infrared light to probe highly scattering media. Typical applications include the monitoring of the oxygenation state of blood in the neonatal brains, or the detection of breast cancer, see [2, 11, 17, 18].

The transport of light in highly scattering media is usually modeled by the diffusion approximation, which can be derived from moment expansions of the underlying, more basic radiative transfer equation [5, 2]. In case of continuous or intensity modulated excitation, this yields an elliptic boundary value problem describing mathematically the physics of light propagation in the sample of interest.

The inverse problem of optical tomography then consist of determining the distribution of optical parameters from measurements of the transmitted light at the boundary. Uniqueness of solutions can be proved, if intensity modulated light is used for the excitation [19, 12, 16], but also non-uniqueness results are known, if one tries to simultaneously identify the distribution of absorption and diffusion coefficients using continuous wave excitation measurements [19, 3].

Since the mapping that associates optical parameters to measurements is compact (with respect to all reasonable topologies), the inverse problem is ill-posed. Therefore, some regularization method has to be used, in order to obtain stable solutions, in particular in the presence of measurement perturbations.

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In this paper, we investigate the applicability of Tikhonov regularization, and also comment on the use of iterative regularization methods in remarks. In order to be able to apply standard results from regularization theory for nonlinear inverse problems, we have to investigate in detail the properties of the forward operator (the mapping of parameters to measurements).

Forward operators in optical tomography have been investigated previously in [8]; see also [23] for related results in impedance tomography. In these works, Banach space topologies $(L^{\infty} \text{ or } L^p, p > 2)$ are used in the parameter space, which simplifies the analysis of the forward operators considerably. In particular, using the L^{∞} -norm for the parameters, as in [8], continuity and Fréchet differentiability of the forward operator follow almost trivially. From a numerical point of view, it is however advantageous to utilize Hilbert space topologies for the parameter and measurement spaces, and we will adopt such an approach here. This does not only facilitate the analysis of (the regularized solution of) the inverse problem, but also simplifies the discretization and numerical solutions of the resulting nonlinear (optimization) problems. The results of [8, 23] are not applicable to the setting investigated here; in fact, we require a much more detailed analysis of the governing boundary value problems. Our results are based on certain $W^{1,p}$ a-priori estimates for solutions to the governing elliptic boundary value problem, which we establish under mild assumptions on the coefficients and the smoothness of the domain. Having developed such a detailed analysis of the forward operator, the standard convergence results for nonlinear Tikhonov regularization can be derived easily with the usual arguments.

The outline of the manuscript is as follows: After fixing the relevant notation, we introduce in Section 2 the boundary value problem governing diffuse transport of light in tissue, and define the forward operator, that maps optical parameters to virtual boundary measurements. In Section 3, we investigate in detail the properties of this forward operator, i.e., we derive continuity and differentiability results, and show compactness and weakclosedness, which are central properties for the regularization of the inverse problem. In Section 4, we then formally introduce the inverse problem, and its regularization, and we summarize the basic convergence results, which follow easily from the results of Section 3. A derivation of regularity results for solutions to elliptic boundary value problems, which are required for our analysis, is given in the appendix.

2. Basic notation and the physical model

2.1. Basic notation and preliminaries. Throughout the text, $\Omega \subset \mathbb{R}^d$, d = 2, 3 will denote a domain with (at least) Lipschitz regular boundary. For $1 \leq p < \infty$, we denote by $L^p(\Omega)$ the standard Lebesgue space of power-p integrable (real or complex valued) functions with norm $||f||_{p;\Omega}^p = \int_{\Omega} |f(x)|^p dx$. The space $L^{\infty}(\Omega)$ of essentially bounded functions is equipped with the norm $||u||_{\infty;\Omega} = \operatorname{ess\,sup}_{x\in\Omega} |u(x)|$, and the scalar product $(u, v)_{\Omega} := \int_{\Omega} u \,\overline{v} \, dx$, is used for the Hilbert space $L^2(\Omega)$. By $W^{1,p}(\Omega)$, we denote the usual Sobolev space equipped with the norm $||u||_{1,p;\Omega}^p = ||u||_{p;\Omega}^p + ||\nabla u||_{p;\Omega}^p$. The space $H^1(\Omega) := W^{1,2}(\Omega)$ with scalar product $(u, v)_{1,\Omega} := (u, v)_{\Omega} + (\nabla u, \nabla v)_{\Omega}$

is again a Hilbert space. Spaces, norms, and scalar products for functions defined on the boundary $\partial \Omega$ are defined accordingly.

We will frequently make use of the following embedding theorems; for proofs and general material on Sobolev spaces, we refer to the book by Adams [1].

Theorem 2.1 (Embedding theorems). (A) The embedding $W^{1,p}(\Omega) \to L^q(\Omega)$ is continuous if (i) d > p and $q \leq dp/(d-p) =: p^*$ or (ii) $d \leq p$ and $1 < q < \infty$. For (i) with $q < p^*$ or (ii), the embeddings are compact.

(B) The embedding (trace map) $W^{1,p}(\Omega) \to L^r(\partial\Omega)$ is continuous if (i) d > pand $r \leq (d-1)p/(d-p) =: p^{\circ}$ or (ii) $d \leq p$ and $1 < r < \infty$. Again, for (i) with $r < p^{\circ}$ or (ii), the embedding is compact.

Throughout the text, C will denote a generic constant, whose value may may depend on the context.

2.2. Physical model and basic assumptions. The propagation of intensity modulated light in highly scattering media can be described by the diffusion approximation [2]

(1)
$$-\operatorname{div}(\kappa \nabla \Phi) + (\mu + ik)\Phi = 0 \quad \text{in } \Omega,$$

where Φ is the complex amplitude of the photon density, μ is the absorption rate per unit length and $k = \omega/c$ is the wavenumber with ω the modulation frequency and c the speed of light. The photon diffusion coefficient is given by $\kappa = 1/(d \ (\mu + \mu'_s))$ where μ'_s is the reduced scattering rate per unit length, and d is the spatial dimension. The system is completed with Robin boundary conditions [22]

(2)
$$\kappa \partial_n \Phi = \rho \left(q - \Phi \right)$$
 on $\partial \Omega$,

which model a diffuse light source located at the boundary. The positive parameter function ρ allows to take into account a refractive index mismatch between Ω and the surrounding space [14].

In order to ensure solvability of the boundary value problem (1)-(2), we impose the following basic conditions on the coefficients.

Assumption 2.2. (i) The function ρ is uniformly positive and bounded, i.e., there exist positive constants ρ , $\overline{\rho}$ such that $\rho \leq \rho \leq \overline{\rho}$ on $\partial\Omega$.

- (ii) The function κ is uniformly positive and bounded, i.e., there exist $\underline{\kappa}$, $\overline{\kappa} > 0$ such that $\underline{\kappa} \leq \kappa \leq \overline{\kappa}$ on Ω .
- (iii) The function μ ∈ L[∞](Ω) is non-negative and bounded from above,
 i.e., there exists μ such that 0 ≤ μ ≤ μ.

The following result is a special case of Theorem A1, which is based on the the complex version of the Lax-Milgram theorem.

Theorem 2.3. Let Assumption 2.2 hold. Then, for any source $q \in L^2(\partial\Omega)$, the boundary value problem (1)–(2) has a unique (complex-valued) solution $\Phi \in H^1(\Omega)$ that satisfies

$$\|\Phi\|_{1,2;\Omega} \le C \|q\|_{2;\partial\Omega}$$

with a constant C depends only on the domain Ω and the bounds of the coefficients in Assumption 2.2.

2.3. Measurements. The measurable quantity in optical tomography is the complex amplitude of the photon flux leaving the domain Ω , i.e., $\kappa \partial_n \Phi$, which by (2) equals $\rho (q - \Phi)$. By a change of signs, we can define the measurement operator as

(4)
$$B: H^1(\Omega) \to L^2(\partial\Omega), \quad \Phi \mapsto \rho (\Phi - q)|_{\partial\Omega}.$$

The following result is a direct consequence of Theorem 2.1(B), and is stated for later reference.

Lemma 2.4. Let $q \in L^2(\partial \Omega)$ be given and Assumption 2.2 hold. Then the measurement operator $B : H^1(\Omega) \to L^2(\partial \Omega)$ is a bounded, compact, affine linear operator.

Remark 2.5. In practice, the light intensities are measured, e.g., by a digital camera, at finitely many locations. One pixel then integrates the photon flux over some area Γ_i , and the measurement operator may be defined as B^N : $H^1(\Omega) \to \mathbb{C}^N$, $\Phi \mapsto \left[\frac{1}{|\Gamma_i|}\int_{\Gamma_i} (\Phi-q) \, ds\right]_{1 \leq i \leq N}$. Since B^N is obtained from B by projection to a finite dimensional space, and N is typically big, we will mostly consider the idealized case of continuous measurements, and comment on implications for the case of finitely many measurements in remarks. It follows from the Cauchy Schwarz inequality that $\int_{\Gamma_i} (\Phi-q) \, ds \leq |\Gamma_i|^{1/2} ||\Phi-q||_{2;\Gamma_i}$, and hence by Lemma 2.4, B^N is a continuous operator from $H^1(\Omega) \to \mathbb{C}^N$.

2.4. Forward operator. In the following, we define a forward operator, which associates a known distribution of optical parameters κ , μ to the corresponding measurements of the outgoing light. This is the mathematical model for a virtual experiment in optical tomography. For ease of notation, we introduce the set of admissible parameters

(5)
$$\mathcal{D}(F) = \{(\kappa, \mu) \in L^2(\Omega) \times L^2(\Omega) : \text{Assumption 2.2 is satisfied}\}.$$

Definition 2.6 (Forward operator). For a given source $q \in L^2(\partial\Omega)$, let us define the nonlinear mapping

(6)
$$F: \mathcal{D}(F) \to L^2(\partial\Omega), \qquad (\kappa, \mu) \mapsto B(\Phi),$$

where Φ denotes the solution of the elliptic boundary value problem (1)–(2).

Due to Theorem 2.3 and Lemma 2.4, the forward operator is well defined.

Remark 2.7. For ease of presentation, we consider only the case of one excitation q here, but the gerenalization to the practically relevant case of finitely many sources is straight forward. One would then define the forward operator as the map $F := (F_{q_1}, \ldots, F_{q_n})$ where F_{q_i} denotes the operator from Definition 2.6 corresponding to the source q_i . Similarly, one can consider the case of finitely many measurements; cf Remark 2.5.

3. PROPERTIES OF THE FORWARD OPERATOR

In this section, we investigate in detail the mapping properties of the forward operator F, i.e., we prove results concerning continuity and compactness, and we derive certain differentiability properties.

3.1. Continuity and compactness of the forward operator. Throughout, we assume that the forward operator $F : \mathcal{D}(F) \to L^2(\partial\Omega)$ is defined according to (1) for some given source term $q \in L^2(\partial\Omega)$. If not stated otherwise, the image and pre-image space of the operator F are equipped with the topologies of $H^1(\Omega) \times L^2(\Omega)$ and $L^2(\partial\Omega)$, respectively. Some of our results however hold with respect to a weaker topology in the parameter space, and we comment on this in remarks.

Remark 3.1. The choice of the $H^1(\Omega) \times L^2(\Omega)$ topology for the parameter space is motivated by the following considerations: The restriction to Hilbert spaces facilitates the analysis, in particular of the inverse problem treated in Section 4; additionally, the norms and scalar proudcts can easily be realized in computations. As will be clear from the analysis below, some additional regularity is required for the parameter κ , in order to obtain the basic properties that are required to ensure, e.g., existence of minimizers in Theorem 4.1, or the Taylor estimate of Theorem 3.17.

Remark 3.2. The set of admissible parameters $\mathcal{D}(F)$ does not contain interior points, i.e., for any $(\kappa, \mu) \in \mathcal{D}(F)$ the ball $B_{\epsilon}(\kappa, \mu) := \{(\tilde{\kappa}, \tilde{\mu}) \in \mathcal{D}(F) :$ $\|\kappa - \tilde{\kappa}\|_{1,2;\Omega}^2 + \|\mu - \tilde{\mu}\|_{2;\Omega}^2 < \epsilon^2\}$ is not completely contained in $\mathcal{D}(F)$ for any $\epsilon > 0$. Therefore, all results stated below have to be understood with respect to the relative topology.

Theorem 3.3 (Continuity). The operator $F : \mathcal{D}(F) \to L^2(\partial\Omega)$ is continuous.

Proof. Let $\{(\kappa_n, \mu_n)\} \subset \mathcal{D}(F)$ be a sequence converging to (κ, μ) in $H^1(\Omega) \times L^2(\Omega)$. Since the set $\mathcal{D}(F)$ is closed, the limit $(\kappa, \mu) \in \mathcal{D}(F)$. Now let Φ_n and Φ denote the (weak) solutions of the boundary value problems (1)–(2) with parameters (κ_n, μ_n) and (κ, μ) , respectively. Since by Theorem 2.3, the solutions Φ_n are uniformly bounded, there exists a weakly convergent subsequence (again denoted by Φ_n) such that $\Phi_n \rightharpoonup y$ weakly in $H^1(\Omega)$ for some $y \in \mathcal{D}(F)$. By linearity of the equations (1)–(2), the difference $w_n := \Phi_n - \Phi$ satisfies for every $v \in C^{\infty}(\overline{\Omega})$ the equation

(7)
$$(\kappa \nabla w_n, \nabla v)_{\Omega} + ((\mu + ik)w_n, v)_{\Omega} + (\rho w_n, v)_{\partial\Omega}$$
$$= ((\kappa_n - \kappa)\nabla \Phi_n, \nabla v)_{\Omega} + ((\mu_n - \mu)\Phi_n, v)_{\Omega} =: (*).$$

Using the Cauchy-Schwarz and Hölder inequalities, we further obtain

 $|(*)| \le \|\kappa_n - \kappa\|_{2;\Omega} \|\nabla \Phi_n\|_{2;\Omega} \|\nabla v\|_{\infty;\Omega} + \|\mu_n - \mu\|_{2;\Omega} \|\Phi_n\|_{2;\Omega} \|v\|_{\infty;\Omega}.$

Thus, convergence of $\kappa_n \to \kappa$ in $H^1(\Omega)$ and $\mu_n \to \mu$ in $L^2(\Omega)$ imply convergence of the right-hand side of (7) to zero. The weak limit $w = y - \Phi$ then is a solution of the variational problem

$$(\kappa \nabla w, \nabla v)_{\Omega} + ((\mu + ik)w, v)_{\Omega} + (w, v)_{\Omega} = 0,$$

and by density of $C^{\infty}(\overline{\Omega})$ in $H^1(\Omega)$ and Theorem 2.3, we obtain $w \equiv 0$. This shows that $\Phi_n \to \Phi$ weakly in $H^1(\Omega)$, and by the definition of F and the compactness of the measurement operator B, we obtain that $F(\kappa_n, \mu_n) \to$ $F(\kappa, \mu)$ strongly in $L^2(\partial \Omega)$ (for this subsequence). Note that the same arguments hold for any subsequence of $\{\Phi_n\}$, which proves the result. \Box *Remark* 3.4. A careful inspection of the previous proof shows that F is continuous also with respect to the weaker topology of $L^2(\Omega) \times L^2(\Omega)$ for the parameter space.

Corollary 3.5 (Compactness). The operator $F : \mathcal{D}(F) \to L^2(\partial\Omega)$ is compact.

Proof. The compactness follows directly from the proof of the previous result and the compactness of the measurement operator B.

As we will show below, the inverse problem of optical tomography is illposed due to the compactness of the forward operator F. In order to apply standard results of regularization theory, we will require the following basic properties.

Theorem 3.6 (Weak closedness). The operator $F : \mathcal{D}(F) \to L^2(\partial\Omega)$ is (sequentially) closed with respect to the weak topologies of $H^1(\Omega) \times L^2(\Omega)$ and $L^2(\partial\Omega)$, i.e., if $(\kappa_n, \mu_n) \to (\kappa, \mu)$ weakly in $H^1(\Omega) \times L^2(\Omega)$, then $(\kappa, \mu) \in \mathcal{D}(F)$ and $F(\kappa_n, \mu_n) \to F(\kappa, \mu)$ weakly in $L^2(\partial\Omega)$.

Proof. Since $\mathcal{D}(F)$ is closed and convex, it is weakly closed [24, Thm 3.12], and consequently the weak limit $(\kappa, \mu) \in \mathcal{D}(F)$. Due to the compact embedding of $H^1(\Omega) \hookrightarrow L^2(\Omega)$, we have $\kappa_n \to \kappa$ (strongly) in $L^2(\Omega)$. Moreover, using the notation of the proof of Theorem 3.3, we obtain that $\Phi_n \to \Phi$ in $L^2(\Omega)$ and thus $((\mu_n - \mu)\Phi_n, v)_{\Omega} \to 0$ (see (7)). It then follows from Remark 3.4 that $F(\kappa_n, \mu_n) \to F(\kappa, \mu)$ strongly in $L^2(\partial\Omega)$.

As the proof of the previous theorem reveals, the operator F actually maps weakly converging sequences in $H^1(\Omega) \times L^2(\Omega)$ to strongly convergent sequences in $L^2(\partial\Omega)$.

Corollary 3.7. The operator $F : \mathcal{D}(F) \to L^2(\partial\Omega)$ is completely continuous, i.e., if $(\kappa_n, \mu_n) \rightharpoonup (\kappa, \mu)$ weakly in $H^1(\Omega) \times L^2(\Omega)$ then $F(\kappa_n, \mu_n) \to F(\kappa, \mu)$ strongly in $L^2(\partial\Omega)$.

Remark 3.8. The two previous results essentially rely on the compact embedding of $H^1(\Omega) \hookrightarrow L^2(\Omega)$, which is used to obtain strong convergence of $\kappa_n \to \kappa$ in $L^2(\Omega)$. In fact, the results derived so far remain valid, if other spaces that are compactly embedded in $L^2(\Omega)$ are used for defining an appropriate weak topology in the parameter space.

3.2. Hölder and Lipschitz continuity. In the following, we derive Hölder and Lipschitz continuity results for the forward operator. For proving these properties, we require some additional regularity of solutions to the governing boundary value problem (1)-(2). The basis for our results is a theorem due to Meyers [21], which states that the (weak) solution of the problem

$$\operatorname{div}(\kappa \nabla u) = \operatorname{div}(f) + g \qquad \text{in } \Omega,$$

lies in $W^{1,p}(\Omega)$ whenever $f \in L^p(\Omega, \mathbb{R}^d)$ and $g \in L^q(\Omega)$, $q' = (p')^\circ$ for some p > 2 depending on the domain Ω and the bounds for the parameter κ . The following result, which is proven in detail in the appendix, can then be derived by perturbation arguments. For ease of notation, let us define for $1 the dual index <math>p' := \frac{p}{p-1}$, and $\bar{p} := ((p')^*)'$, $\hat{p} := ((p')^\circ)'$, where p^* , p° are as in Theorem 2.1.

 $\mathbf{6}$

Theorem 3.9. Let Assumption 2.2 hold. Then there exists a constant $p_0 > 2$ depending only on the domain and the bounds for the coefficients, such that the solution u of the variational problem

(8)

$$(\kappa \nabla u, \nabla v)_{\Omega} + ((\mu + ik)u, v)_{\Omega} + (\rho u, v)_{\partial\Omega}$$

$$= (f, \nabla v)_{\Omega} + (g, v)_{\Omega} + (\rho q, v)_{\partial\Omega} \qquad \text{for all } v \in C^{\infty}(\overline{\Omega}),$$

lies in $W^{1,p}(\Omega)$ whenever $f \in L^p(\Omega, \mathbb{R}^d)$, $g \in L^{\bar{p}}(\Omega)$, and $q \in L^{\hat{p}}(\partial\Omega)$ for some $\frac{p_0}{p_0-1} \leq p \leq p_0$. Moreover, there holds the a-priori estimate

$$||u||_{1,p;\Omega} \le C(||f||_{p;\Omega} + ||g||_{\bar{p};\Omega} + ||q||_{\hat{p};\partial\Omega})$$

with a constant C that depends only on Ω and the bounds for the coefficients. If the domain Ω has a smooth boundary, and if $\overline{\kappa}/\underline{\kappa}$ approaches one, then the maximal p_0 such that the statement of the theorem holds, tends to infinity.

Remark 3.10. The indices \bar{p} , \hat{p} arise from Hölder's inequality and embedding theorems. For dimension d = 2 and p > 2 we have $\bar{p} = 2p/(2+p)$ and $\hat{p} = p/2$. Similarly, for d = 3 and p > 3/2 there holds $\bar{p} = 3p/(3+p)$ and $\hat{p} = 2p/3$. If d = 2 and $p \le 2$, or d = 3 and $p \le 3/2$, then \bar{p} , \hat{p} can be chosen to be any number in $(1, \infty)$.

As a first consequence of this theorem, we obtain a uniform regularity result for solutions of the forward problem (1)-(2).

Corollary 3.11. Let Assumption 2.2 hold, and let Φ denote the solution of (1)–(2) for some $q \in L^2(\partial\Omega)$. Then $\Phi \in W^{1,p}(\Omega)$ for some p > 2, and there holds the uniform bound $\|\Phi\|_{1,p;\Omega} \leq C \|q\|_{2;\partial\Omega}$ with a constant C depending only on the domain and the bounds for the coefficients. The estimate holds, in particular, for every $3/2 \leq p \leq 3$, if Ω is smooth and $\overline{\kappa}/\underline{\kappa}$ is sufficiently close to one.

Proof. The assumption $q \in L^2(\partial\Omega)$ implies the condition $\hat{p} \leq 2$, which in view of Remark 3.10 yields the restriction $p \leq 3$ for d = 2, 3 space dimensions; the lower bound arises from duality arguments. The result then follows from Theorem 3.9 and Remark 3.10. Note that the bounds on p could be relaxed, if q is assumed to be more regular.

Using this a-priori result on regularity of solutions Φ , we can specify the continuous dependence of the solution Φ on the parameters κ and μ more precisely.

Theorem 3.12. Let Assumption 2.2 hold, and let Φ and Φ denote the solutions of (1)–(2) with $q \in L^2(\partial\Omega)$ for parameters (κ, μ) and $(\tilde{\kappa}, \tilde{\mu})$, respectively. Then

$$\|\tilde{\Phi} - \Phi\|_{1,2;\Omega} \le C \big(\|\tilde{\kappa} - \kappa\|_{1,2;\Omega}^{\eta} + \|\tilde{\mu} - \mu\|_{2;\Omega} \big) \|q\|_{2;\partial\Omega},$$

with a constant C depending only on the bounds of the parameters and the domain. The Hölder index is given by $\eta = \min\{(3p-6)/p, 1\}$ with p from Corollary 3.11.

Proof. Let us define $\delta \kappa := \tilde{\kappa} - \kappa$ and $\delta \mu := \tilde{\mu} - \mu$. Then $w := \tilde{\Phi} - \Phi$ satisfies $(\kappa \nabla w, \nabla v)_{\Omega} + ((\mu + ik)w, v)_{\Omega} + (\rho w, v)_{\partial\Omega} = -(\delta \kappa \nabla \tilde{\Phi}, \nabla v)_{\Omega} - (\delta \mu \; \tilde{\Phi}, v)_{\Omega}$

for all $v \in H^1(\Omega)$. By continuous embedding of $H^1(\Omega) \hookrightarrow L^6(\Omega)$ (in d = 2, 3 space dimensions) and noting that $\|\tilde{\Phi}\|_{1,p;\Omega} \leq C \|q\|_{2;\partial\Omega}$ for some p > 2 by Corollary 3.11, we obtain by Hölders inequality

$$\|\delta\kappa\nabla\Phi\|_{2;\Omega} \le \|\delta\kappa\|_{2p/(p-2);\Omega}\|\Phi\|_{1,p;\Omega}, \quad \|\delta\mu \ \Phi\|_{5/6;\Omega} \le \|\delta\mu\|_{2;\Omega}\|\Phi\|_{1,2;\Omega}.$$

If p = 3, then $\|\delta\kappa\|_{2p/(p-2);\Omega} \leq \|\delta\kappa\|_{6;\Omega} \leq C \|\delta\kappa\|_{1,2;\Omega}$, and the results follows with $\eta = 1$. For $2 \leq p \leq 3$, we obtain by interpolation

$$\|\delta\kappa\|_{2p/(p-2);\Omega} \le C'\overline{\kappa}^{\frac{6-2p}{p}} \|\delta\kappa\|_{6;\Omega}^{\frac{3p-6}{p}} \le C\|\delta\kappa\|_{1,2;\Omega}^{\frac{3p-6}{p}},$$

which yields the result with $\eta = 3(p-2)/p$. Note that for $p \to 3$ the index η tends to one, and $\eta \to 0$ for p tending to 2.

Corollary 3.13 (Hölder continuity). Let the assumptions of Theorem 3.12 hold. Then the forward operator $F : \mathcal{D}(F) \to L^2(\partial\Omega)$ is Hölder continuous with respect to the topologies of $H^1(\Omega) \times L^2(\Omega)$ and $L^2(\partial\Omega)$.

Corollary 3.14 (Lipschitz continuity). Let the assumptions of Theorem 3.12 hold. If d = 2, or if d = 3 and additionally Ω is smooth and $\overline{\kappa}/\underline{\kappa}$ is sufficiently close to one, then F is Lipschitz continuous with respect to the topologies of $H^1(\Omega) \times L^2(\Omega)$ and $L^2(\partial\Omega)$.

Proof. For space dimension d = 2, we have $H^1(\Omega) \hookrightarrow L^r(\Omega)$ for all $1 < r < \infty$, which allows us to estimate $\|\delta\kappa\|_{2p/(p-2);\Omega} \leq C \|\delta\kappa\|_{1,2;\Omega}$, and the result follows along the lines of the proof of Theorem 3.12. The Lipschitz continuity for d = 3 follows directly from Theorem 3.12, and the mapping properties of the measurement operator B.

3.3. Results on differentiability. The Lipschitz continuity of the forward operator F indicates, that a certain differentiability might be expected. Since differentiability is a key property for the convergence of iterative algorithms for the solution of nonlinear operator equations, as well as for the derivation of quantitative estimates in regularization theory, we will derive some results in this direction. For the following considerations, we assume that d = 2, or that d = 3 and additionally Ω is smooth and $\overline{\kappa}/\underline{\kappa}$ is sufficiently close to one, such that the forward operator is Lipschitz continuous, cf Corollary 3.14.

Theorem 3.15 (Differentiability). Let $q \in L^2(\partial\Omega)$ be given, and let $(\kappa, \mu) \in \mathcal{D}(F)$ and $(\delta\kappa, \delta\mu) \in H^1(\Omega) \times L^2(\Omega)$ such that $(\kappa + t\delta\kappa, \mu + t\delta\mu) \in \mathcal{D}(F)$ for all $t \in \mathbb{R}$ with |t| sufficiently small. Then the derivative of F at (κ, μ) in direction $(\delta\kappa, \delta\mu)$ is given by $F'(\kappa, \mu)[\delta\kappa, \delta\mu] = \rho w|_{\partial\Omega}$, where w solves the sensitivity problem

(9)

 $(\kappa \nabla w, \nabla v)_{\Omega} + ((\mu + ik)w, v)_{\Omega} + (\rho w, v)_{\partial \Omega} = -(\delta \kappa \nabla \Phi, \nabla v)_{\Omega} - (\delta \mu \Phi, v)_{\Omega}$

for all $v \in H^1(\Omega)$, and Φ denotes the solution of (1)–(2). Moreover, there holds the uniform estimate

(10) $\|F'(\kappa,\mu)[\delta\kappa,\delta\mu]\|_{2;\partial\Omega} \le C(\|\delta\kappa\|_{1,2;\Omega} + \|\delta\mu\|_{2;\Omega})\|q\|_{2;\partial\Omega}$

with a constant C depending only on Ω and the bounds of the coefficients.

Proof. The result follows similarly to Theorem 3.12 and Corollary 3.14. \Box

Theorem 3.16. Let the assumptions of Theorem 3.15 hold. Then $F'(\kappa, \mu)[\delta\kappa, \delta\mu]$ defines a bounded linear operator $F'(\kappa, \mu) : H^1(\Omega) \times L^2(\Omega) \to L^2(\partial\Omega)$, and the estimate (10) holds for all $(\delta\kappa, \delta\mu) \in H^1(\Omega) \times L^2(\Omega)$.

Proof. The set $B_{\epsilon}(\kappa,\mu) \cap \mathcal{D}(F)$ is dense in $B_{\epsilon}(\kappa,\mu) := \{(\tilde{\kappa},\tilde{\mu}) : \|\tilde{\kappa}-\kappa\|_{H^{1}(\Omega)}^{2} + \|\tilde{\mu}-\mu\|_{L^{2}(\Omega)}^{2} \leq \epsilon^{2}\}$, and thus $F'(\kappa,\mu)$ is densly defined by the directional derivatives, and uniformly bounded by (10). By the uniform boundedness principle there exists a unique continuous extension, again denoted by $F'(\kappa,\mu)$.

For the proof of convergence rates or the convergence of iterative regularization methods, we will utilize the following estimate of the remainder of the linear approximation.

Theorem 3.17. Assume that Ω is smooth, and that either d = 2, or d = 3and $\overline{\kappa}/\underline{\kappa}$ is sufficiently close to one such that Theorem 3.9 holds with $p_0 = 3$. Then the linear Taylor expansion of F around $(\kappa, \mu) \in \mathcal{D}(F)$ is second order accurate, i.e., for $(\tilde{\kappa}, \tilde{\mu}) \in \mathcal{D}(F)$ there holds

$$\begin{aligned} \|F(\tilde{\kappa},\tilde{\mu}) - F(\kappa,\mu) - F'(\kappa,\mu)[\tilde{\kappa}-\kappa,\tilde{\mu}-\mu]\|_{2;\partial\Omega} \\ &\leq C_L \Big(\|\tilde{\kappa}-\kappa\|_{1,2;\Omega}^2 + \|\tilde{\mu}-\mu\|_{2;\Omega}^2\Big) \|q\|_{2;\partial\Omega}, \end{aligned}$$

with a constant C_L depending only on the domain Ω and the bounds for the coefficients in Assumption 2.2.

Proof. Let Φ and $\tilde{\Phi}$ denote the solution of the forward problem (1)–(2) with parameters $(\tilde{\kappa}, \tilde{\mu})$ and (κ, μ) , respectively. Moreover, let w be the solution of (9), and define $\delta \kappa := \tilde{\kappa} - \kappa$ and $\delta \mu := \tilde{\mu} - \mu$. Then the function $z := \tilde{\Phi} - \Phi - w$ satisfies the variational problem

$$\begin{aligned} (\kappa \nabla z, \nabla v)_{\Omega} + ((\mu + ik)z, v)_{\Omega} + (\rho z, v)_{\partial\Omega} \\ &= -(\delta \kappa \nabla (\tilde{\Phi} - \Phi), \nabla v)_{\Omega} - (\delta \mu \ (\tilde{\Phi} - \Phi), v)_{\Omega} \end{aligned}$$

for all $v \in H^1(\Omega)$. Application of Hölder's inequality yields

$$\|\delta\kappa\nabla(\Phi-\Phi)\|_{3/2;\Omega} \le \|\delta\kappa\|_{6;\Omega}\|\Phi-\Phi\|_{1,2;\Omega}.$$

Thus, by Theorem 3.9 with p = 3/2, the solution of this variational problem satisfies $z \in W^{1,3/2}(\Omega)$, and the result follows by Corollary 3.14, the continuous embedding of $H^1(\Omega) \hookrightarrow L^6(\Omega)$, and by the continuity of the trace mapping $W^{1,3/2}(\Omega) \to L^2(\partial\Omega)$ in d = 2, 3 dimensions.

A careful inspection of the previous proof reveals, that the H^1 -topology provides the minimal regularity for the parameter κ in order to obtain the Lipschitz continuity of the derivative. This is an important property for the analysis of the inverse problem presented in the next section.

4. INVERSE PROBLEM

The inverse problem in diffuse optical tomography consists of finding the parameters $(\kappa, \mu) \in \mathcal{D}(F)$ corresponding to the data y^{δ} , i.e., to solve the nonlinear operator equation

(11)
$$F(\kappa,\mu) = y^{\delta}, \quad (\kappa,\mu) \in \mathcal{D}(F), \ y^{\delta} \in L^2(\partial\Omega).$$

Here, y^{δ} denotes the (possibly perturbed) measurement of the true data y, for which the inverse problem is assumed to have a solution for physical reasons; i.e., there exists (κ, μ) such that $F(\kappa, \mu) = y$. Due to the compactness of the forward operator F (cf Corollary 3.5), the inverse problem (11) is illposed, and thus some regularization method has to be used for obtaining stable solutions. In the following, we consider Tikhonov regularization, i.e., we define an approximate solution $(\kappa_{\alpha}^{\delta}, \mu_{\alpha}^{\delta})$ as a minimizer of the Tikhonov functional

(12)
$$J_{\alpha}(\kappa,\mu) := \frac{1}{2} \|F(\kappa,\mu) - y^{\delta}\|^{2} + \frac{\alpha}{2} \left(\|\kappa - \kappa_{0}\|_{1,2;\Omega}^{2} + \|\mu - \mu_{0}\|_{2;\Omega}^{2}\right)$$

in $\mathcal{D}(F)$. The element (κ_0, μ_0) serves as an a-priori guess for the unknown parameters. Choosing a positive regularization parameter $\alpha > 0$ allows to establish existence of minimizers and stability of the solution process. The following results follow with minor modifications from standard regularization theory for nonlinear inverse problems, and we state them without proof. For details and proofs we refer to [10] or [9, Ch 10].

The existence of minimizers, which is required for the well-definedness of the regularization method, is a direct consequence of Theorem 3.6.

Theorem 4.1 (Existence of a minimizer). For any $\alpha > 0$ the Tikhonov functional J_{α} has a minimizer in $\mathcal{D}(F)$.

The next result shows, that the regularized solutions depend continuously on the data, as long as the regularization parameter is strictly positive.

Theorem 4.2 (Stability). Let $\alpha > 0$, and let $\{y_n\}$ be a sequence of data with $y_n \to y$. Moreover, let (κ_n, μ_n) denote minimizers of (12) with y^{δ} replaced by y_n . Then $\{(\kappa_n, \mu_n)\}$ has a convergent subsequence, and the limit of every convergent subsequence is a minimizer of J_{α} in $\mathcal{D}(F)$.

As a next step, we state that the regularized solutions converge, if the perturbations of the data go to zero and the regularization parameter is chosen appropriately.

Theorem 4.3 (Convergence). Let $\{y_n\} \subset L^2(\partial\Omega)$ denote a sequence of data with $||y_n - y|| \leq \delta_n$. If $\delta_n \to 0$ and the regularization parameter is chosen such that $\alpha(\delta_n) \sim \delta_n$, then any sequence of minimizers $\{(\kappa_n, \mu_n)\}$ of the Tikhonov functional (12) with y^{δ} replaced by y_n contains a convergent subsequence, and the limit of every convergent subsequence is a (κ_0, μ_0) -minimum-norm solution of (11).

Remark 4.4. One can show that under additional assumptions on the parameters, the inverse problem of diffuse optical tomography has a unique solution, if measurements are taken for infinitely many excitations, i.e., the full (in our case) Robin-to-Neumann map is measured. For results in this

direction, see [3, 12, 16]. If uniqueness is assumed, then the statement of the previous theorem simplifies, since in this case every subsequence converges to the same limit.

In order to obtain quantitative convergence results, a source condition, i.e., some smoothness of the solution, is required. For stating such a condition, let us introduce the adjoint of the derivative operator $F'(\kappa, \mu)$, cf. Theorem 3.16. The following representation can be derived with standard arguments.

Theorem 4.5. Let $(\kappa, \mu) \in \mathcal{D}(F)$. Then the adjoint of the operator $F'(\kappa, \mu)$ defined in Theorem 3.16 is given by

(13)
$$F'(\kappa,\mu)^*: L^2(\partial\Omega) \to H^1(\Omega) \times L^2(\Omega), \qquad r \mapsto (z,\overline{\Phi}R)$$

where Φ is the solution of the forward problem (1)–(2), R is the solution of the adjoint problem

(14)
$$-\operatorname{div}(\kappa \nabla R) + (\mu - ik)R = 0 \qquad in \ \Omega,$$

(15)
$$\kappa \partial_n R = \rho(r - R)$$
 on $\partial \Omega$,

and $z \in H^1(\Omega)$ is defined by

$$-\Delta z + z = \nabla \overline{\Phi} \nabla R \quad in \ \Omega, \qquad \partial_n z = 0 \quad on \ \partial \Omega.$$

For the following classical convergence rate result, cf. [10] or [9, Thm 10.4], it is usually assumed that F is Fréchet differentiable, with Lipschitz continuous Fréchet derivative. This condition can be replaced by the second order Taylor estimate stated in Theorem 3.17, and we obtain the following quantitative result.

Theorem 4.6. Let $y^{\delta} \in L^2(\Omega)$ with $||y - y^{\delta}|| \leq \delta$, and let the assumptions of Theorem 3.17 hold. Assume that $(\kappa^{\dagger}, \mu^{\dagger})$ is a (κ_0, μ_0) -minimum-norm solution, and that the following conditions hold:

(1) There exists an element $w \in L^2(\partial\Omega)$ such that

$$(\kappa^{\dagger},\mu^{\dagger}) - (\kappa_0,\mu_0) = F'(\kappa^{\dagger},\mu^{\dagger})^* w.$$

(2) There holds $C_L ||q||_{2;\partial\Omega} ||w|| < 1$ with C_L from Theorem 3.17.

Then for the parameter choice $\alpha = \delta$, we obtain the convergence rates

$$\|F(\kappa_{\alpha}^{\delta},\mu_{\alpha}^{\delta})-y^{\delta}\|=O(\delta) \qquad and \qquad \|(\kappa_{\alpha}^{\delta},\mu_{\alpha}^{\delta})-(\kappa^{\dagger},\mu^{\dagger})\|=O(\sqrt{\delta}).$$

Remark 4.7. For a numerical realization, the Tikhonov functional has to be minimized by some iterative algorithm. Alternatively, one might consider iterative regularization methods for the stable solution of (11) right away. Let us mention, that under the conditions of Theorem 4.6, one can show convergence of iterative methods, e.g., the iteratively regularized Gauß-Newton method, cf. [4, Thm 4.1, Thm 4.2] or [20].

5. Summary

In this paper we established a rigorous analysis of the forward problem in diffuse optical tomography. In contrast to previous investigations of mapping properties of the forward operator in optical tomography, or, similarly, in electrical impedance tomography, we only used Hilbert space topologies for the parameter space. This facilitates the numerical realization of the resulting regularization methods, and allows the use of standard iterative algorithms for the solution of the corresponding nonlinear optimization problems. Besides showing the complete continuity of the forward operator, which implies the ill-posedness of the corresponding inverse problem, we also proved weak (sequential) closedness of the operator. This allows the stable solution by Tikhonov regularization (with Hilbert space penalty terms), i.p., the existence of minimizers for the Tikhonov functional is ensured. Moreover, convergence of minimizers towards a solution is guaranteed, if the noise level tends to zero and the regularization parameters are chosen appropriately. We also investigated differentiability of the forward operator, and derived second order estimates for the remainder of the linear Taylor approximation, which allowed to derive quantitative convergence rates estimates. Our reslts also allow to apply iterative (regularization) methods for a numerical solution. For the analysis of the forward operator, we utilized $W^{1,p}$ regularity results for elliptic partial differential equations, which were derived in detail under minimal regularity assumptions on the parameters and the mild smoothness requirements on domain.

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A. Appendix

Let us start with a proof of Theorem 3.9 for the case $p_0 = 2$, and recall the definition of \bar{p} and \hat{p} given before the statement of Theorem 3.9.

Theorem A1. Let $\Omega \subset \mathbb{R}^d$, $d \geq 2$ be a Lipschitz domain, and let Assumption 2.2 hold. Then for every $f \in L^2(\Omega, \mathbb{R}^d)$, $g \in L^{\overline{2}}(\Omega)$, and $q \in L^{\widehat{2}}(\partial\Omega)$, the problem (8) of Theorem 3.9 has a unique solution $u \in W^{1,2}(\Omega)$ that satisfies

$$\|u\|_{1,2;\Omega} \le C(\|f\|_{2;\Omega} + \|g\|_{\bar{2};\Omega} + \|q\|_{\hat{2};\partial\Omega})$$

with a constant C only depending on the domain Ω and the bounds for the coefficients in Assumption 2.2.

Proof. By Hölder's inequality, we have

$$\begin{aligned} (f, \nabla v)_{\Omega} + (g, v)_{\Omega} + (q, v)_{\partial\Omega} | \\ &\leq \|f\|_{2;\Omega} \|v\|_{1,2;\Omega} + \|g\|_{(2^*)';\Omega} \|v\|_{2^*;\Omega} + \|q\|_{(2^\circ)';\partial\Omega} \|v\|_{2^\circ;\partial\Omega}, \end{aligned}$$

and application of embedding theorems (cf. Theorem 2.1), shows that the right hand side of (8) defines a bounded linear functional on $H^1(\Omega)$. The result then follows from the complex version of the Lax-Milgram Theorem [7, Ch VII].

In order to generalize this theorem to the case $p_0 > 2$, we need the following basic results, which are a generalization of $W^{1,p}$ regularity results for Dirichlet problems [21, 26] to Neumann boundary conditions. **Theorem A2.** Let $\Omega \subset \mathbb{R}^d$, $d \geq 2$ denote a domain with $\partial \Omega \in C^{1,1}$. Then for every $f \in L^p(\Omega, \mathbb{R}^d)$ and $g \in L^{\bar{p}}(\Omega)$, the problem

(16) $(\nabla u, \nabla v)_{\Omega} + (u, v)_{\Omega} = (f, \nabla v)_{\Omega} + (g, v)_{\Omega}$ for all $v \in C^{\infty}(\overline{\Omega})$

has a unique solution $u \in W^{1,p}(\Omega)$ that satisfies

(17) $||u||_{1,p;\Omega} \le C(||f||_{p;\Omega} + ||g||_{\bar{p};\Omega})$

with a constant $C = C(p, \Omega)$ which is independent of the data f and g.

Proof. According to [25, Theorem 3.1] there exists a constant $C = C(p, \Omega)$ such that

$$||u||_{1,p;\Omega} \le C(||\Delta u||'_{-1,p;\Omega} + ||u||_{p;\Omega})$$

for all functions $u \in C^{\infty}(\overline{\Omega})$. Here $\|\cdot\|'_{-1,p;\Omega}$ denotes the norm of the dual space $\widetilde{W}^{-1,p}(\Omega) := (W^{1,p'}(\Omega))'$. The result then follows by continuous embedding of Sobolev spaces, cf. Theorem 2.1.

Remark A3. The previous result is based on $W^{2,p}$ -regularity of solutions of the Neumann problem $-\Delta u + u = f$, cf. [13, Prop 2.5.2.3], which requires a $C^{1,1}$ boundary. The estimate (17) can then be derived by interpolation arguments, cf [25]. In view of the results of [26, Theorem 4.6], we conjecture, that a C^1 -regular boundary should be sufficient for the result to hold.

The following results are derived with the arguments of [15], where nonlinear mixed boundary value problems were considered. In order to keep track of the assumptions and constants, we carry out the derivations in detail for our linear problem.

Due to Theorem A2, the mapping $J: W^{1,p}(\Omega) \to \widetilde{W}^{-1,p}(\Omega)$ defined by $\langle Ju, v \rangle := \int_{\Omega} \nabla \overline{u} \nabla v + \overline{u}v \, dx$ for $v \in W^{1,p'}(\Omega)$ is an isomorphism, and the norm of its inverse is given by

 $M_p := \sup\{ \|u\|_{1,p;\Omega} : u \in W^{1,p}(\Omega), \ \|Ju\|'_{-1,p} \le 1 \}.$

Note that by the Riesz representation theorem $M_2 = 1$. The linear mapping $L: W^{1,p}(\Omega) \to Y_p := L^p(\Omega, \mathbb{R}^{d+1}), u \mapsto (u, \nabla u)$ is continuous. By identifying Y_p with its dual, the adjoint L^* maps Y_p continuously into $\widetilde{W}^{-1,p}(\Omega)$, and there holds $J = L^*L$. Let us define $A: W^{1,p}(\Omega) \to \widetilde{W}^{-1,p}(\Omega)$ by $\langle Au, v \rangle := \int_{\Omega} \kappa \nabla \overline{u} \nabla v + c \overline{u} v \, dx$ for $v \in W^{1,p'}(\Omega)$ with constant $c := \sqrt{\kappa \overline{\kappa}}$.

Theorem A4. Let Ω be of class $C^{1,1}$. If $l := \frac{\overline{\kappa} - \underline{\kappa}}{\underline{\kappa} + \overline{\kappa}} < 1/M_p$, then A is an isomorphism between $W^{1,p}(\Omega)$ and $\widetilde{W}^{-1,p}(\Omega)$. In particular, for every $h \in \widetilde{W}^{-1,p}(\Omega)$, the variational problem

 $\langle Au, v \rangle = \langle h, v \rangle$ for all $v \in W^{1,p'}(\Omega)$

has a unique solution $u \in W^{1,p}(\Omega)$ that satisfies $||u||_{1,p;\Omega} \leq C ||h||'_{-1,p;\Omega}$ with constant C depending only on Ω , p, and the bounds on the coefficients.

Proof. Compare to the proof of [15, Thm 1]. For $t = \frac{2}{\overline{\kappa} + \underline{\kappa}}$, the operator $T: Y_p \to Y_p, y = (y_0, y') \mapsto y - t(cy_0, \kappa y')$ is Lipschitz continuous with constant $l < 1/M_p$; moreover, there holds $L^*TL = J - tA$. The mapping $Q_h : W^{1,p}(\Omega) \to W^{1,p}(\Omega)$ defined by $Q_h u := J^{-1}(L^*TLu + th) = u - tJ^{-1}(Au - h)$ satisfies $\|Q_h u_1 - Q_h u_2\|_{1,p;\Omega} \leq M_p l \|u_1 - u_2\|_{W^{1,p}(\Omega)}$; i.e., Q_h is Lipschitz

continuous with Lipschitz constant $lM_p < 1$ (independent of h). The result then follows with Banach's fixed point theorem.

Remark A5. Even for non-smooth domains, the result holds at least for some p > 2; cf. [15]. Note that l < 1, and thus $lM_p < 1$ for p sufficiently close to 2 since $M_p \to 1$ as $p \to 2$.

Proof of Theorem 3.9. The problem of Theorem 3.9 can be written as

$$(\kappa \nabla u, \nabla v)_{\Omega} + c(u, v)_{\Omega} = ((c - \mu - ik)u, v)_{\Omega} - (\rho u, v)_{\partial\Omega} + (f, \nabla v)_{\Omega} + (g, v)_{\Omega} + (\rho q, v)_{\partial\Omega} =: \langle h, v \rangle,$$

where $c := \sqrt{\kappa_{\underline{\kappa}}}$ is defined as above. Let us consider the case $2 \leq p \leq 3$ first (which is the relevant case for the analysis of Section 3), and assume that the conditions of Theorem A4 hold. It remains to show that h is a bounded linear functional on $W^{1,p'}(\Omega)$ that can be estimated appropriately. By Hölder's inequality and embedding theorems (cf. Theorem 2.1), we obtain

$$\begin{aligned} |\langle h, v \rangle| &\leq C'(\|u\|_{6;\Omega} + \|u\|_{4;\partial\Omega} + \|f\|_{p;\Omega} + \|g\|_{\bar{p};\Omega} + \|q\|_{\hat{p};\partial\Omega})\|v\|_{1,p';\Omega} \\ &\leq C(\|f\|_{p;\Omega} + \|g\|_{\bar{p};\Omega} + \|q\|_{\hat{p};\partial\Omega})\|v\|_{1,p';\Omega}, \end{aligned}$$

where the last inequality follows from Theorem A1. The result then follows from Theorem A4. Having established this higher regularity of solutions u, the case p > 3 can be treated by a boot-strapping argument. The case $p \le 2$ follows with the standard duality arguments. Thus for smooth domains, and $\overline{\kappa}/\underline{\kappa}$ sufficiently close to 1, Theorem 3.9 holds for any $p_0 < \infty$. For nonsmooth domains, or $\overline{\kappa} \gg \underline{\kappa}$, the theorem follows from the results of [15] and Remark A5 at least for some $p_0 > 0$.

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